

Hydrothermal Synthesis and Structural Determination of NaMnPO₄

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Beamline(s): X7B

Introduction: As a part of design of structures built up from octahedra and tetrahedra building units, the relationship between the structures of manganese phosphates and the synthetic conditions was investigated.

Methods and Materials: Manganese Phosphates can be obtained from mixed solutions of Mn^{2+} , PO_4^{3-} , and MnO_4^- by hydrothermal methods. The mole ratios between reagents, with or without additives such as 2-butanol and tetraalkyl-ammonium ions, and autoclaving temperature have strong influence upon the products obtained. Single crystals of sodium manganese phosphate NaMnPO_4 are prepared when very small amounts of 2-butanol and MnO_4^- are added with autoclaving at 180 °C. The structure of this NaMnPO_4 was resolved from X-ray diffraction data collected at NSLS beamline X7B with a 50 X 50 X 30 μm crystal.

J. Moring *et al.*, have also synthesized NaMnPO_4 with conventional solid state methods at 420 °C.

Results: Sodium manganese phosphate NaMnPO_4 prepared by two different methods has the same structure. All manganese ions have an elongated octahedral environment. As shown in **Figure 1** and **Figure 2**, MnO_6 octahedra share two edges to form a single chain along the [010] direction. The chains are connected by PO_4 tetrahedra via corner-sharing in both [100] and [001] directions to form a 3-dimensional network.

Conclusions: Depending on the synthetic conditions, manganese phosphates with various manganese oxidation states can be prepared via hydrothermal methods.

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References: J. Moring *et al.*, J. Solid State Chem. **61**, 39 (1986), S. Geller *et al.*, Acta Cryst. **13**, 325 (1960)

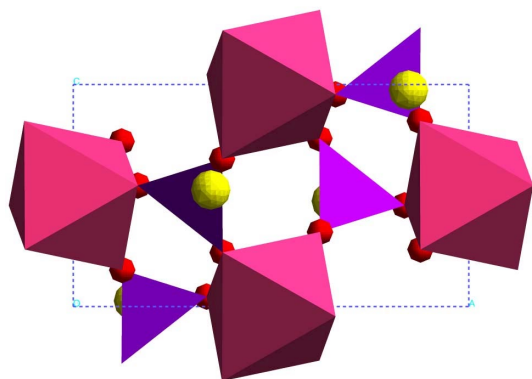


Figure 1. View down b axis. MnO_4 chains connected by PO_4 tetrahedra Na ions yellow.

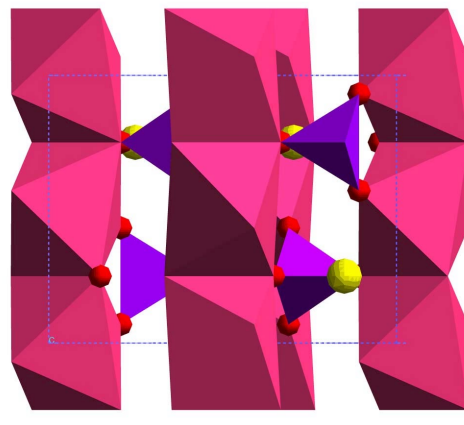


Figure 2. View down c axis. MnO_4 chains connected by PO_4 tetrahedra.